Subject index

Aluminoborane 53
Analytic energy second derivatives 113
Appearance potential 125
Atomic Li 373

Basis set 195
Basis set superposition error (BSSE) 195
Benzenoid hydrocarbon 437
Bond functions 195
Boranes 125
Brillouin conditions 95

Cacti lattices 315
CASSCF 33
Cation complexes 297
s-Character 291
Characteristic polynomials 153, 315
C—H coupling 291
CI 33, 53
CO_2-HF complex 173
Concurrency or multiprocressing 187
Conformational energy maps 377
Coronene 153
Coset representation 247
Counterpoise correction 297
Coupled pair 213
Cyclobutadiene 153
Cyclooctatetraene 153

Delocalization effects 291
Density functional theory 373
Diborane 53
Diboranes 125
Dimer statistics 315
Double perturbation theory 391

Eigenvalue 153
Electric field gradient 285
Electronic structures 125
Electrostatic interaction energy 85
Energy derivatives 227
Enumeration of chemical isomers 47
Enumeration of compounds 247

First-order CASSCF 95
First row atoms 73

Franck-Condon overlap 137
Full CI wave functions

Gaussian basis sets 73
Gaussian computation 285
Generalized perturbed eigenvalue equation 331
Generating function 47
Gradient extremal path 7
Graph spectrum 437
Graph theory 315, 423

H_2^+ 391
Hückel theory 437
Hydrogen bonding 173
Hydrogen persulfide 411
Hydrogen scrambling 53

Interaction energy analysis 297
Internal rotation 411
Iron-ethylene 33

Langrangian formulation 227
Ligand field theory 269
Low rank perturbation 331

Molecular scattering 353
Molecular shape 377
Molecular vibrations 7
Møller-Plesset 227
MRSDCI 213

NMR 291
N_2O-HF complex 173
Nonbonding molecular orbitals 65
Non-canonical basis 227
Non-Hermitian matrices 331
Non-linear expression 213
Non-separable vibrations 137

Organic radicals 65

Pairwise additive function counterpoise (PAFC) 195
Piecewise local perturbations 331

Polarizability of H 391
Polarization wave function 73
Pseudopotential 1

Quadrupole correction 213
Quantum simulation 137

Reaction coordinate 7
Reaction coordinates 353
Reaction graphs 423
Reaction network 423
Reaction path 7
Reactive scattering 353
Related positive ions 125
Relativistic corrections 391
Renormalization of single excitations 95
Rotational isomerism 411
Rydberg states 373

Series analysis 47
Shape invariance maps 377
Site-site function counterpoise (SSFC) 195
Size consistent 213
Spin density 73
Subspectral 153
Subspectrality 437
Successive reaction counterpoise (SRCP) 195
Symmetry adapted functions 269

Table of marks 247
Thermochemical properties 125
Thermodynamic stability 53
Topological method 65
Torsional potential 411
Transition metal complex 33
Two-electron transformation 187

Unitary group approach 269
Unit subduced cycle index 247

Valence-electron-only SCF 1
van der Waals surfaces 377
Vectorization 187